Supplementary Information for “Rapid mixing of sub-microliter drops by magnetic micro-stirring”

Estimate of temperature increase of drop due to viscous dissipation during mixing

The rotating external magnetic field provides energy and does work to rotate the stir bar inside the drop, against the drag force. First the drag force F_d is estimated, and from it the viscous energy dissipated. The drag equation:

$$F_d = \frac{1}{2}\rho v^2 C_D A$$

ρ is the density of the fluid (1000 kg/m^3 for water or an aqueous protein solution), v the velocity of the moving bar, C_D the drag coefficient and A the reference area (projected area in the direction perpendicular to the velocity). For a ‘worst case’ (highest energy dissipated) we assume the bar is oriented with its largest surface area perpendicular to the flow. This results in the highest drag coefficient (about 2 for a long, flat plate, see ref. Hoerner). The spinning speed is 1000 rpm and the bar is estimated to move around a circular trajectory inside the drop of radius 400 µm, giving its velocity v = 2π(1000/60s) x 400µm = 0.042 m/s.

This results in a drag force

$$F_d = 1/2 \text{ x } 1000\text{kg/m}^3 \text{ x } (0.042\text{m/s})^2 \text{ x } 2 \text{ x } (400 \text{ x } 200 \text{ x } 10^{-12} \text{ m}^2) = 141\text{nN}$$

The total work W done during 1 second of mixing (1000/60= 16.7 revolutions happen during that time) is then:

$$W = 2\pi \text{ x } 400\mu\text{m x } 1.4\mu\text{N x } 16.7 = 5.9\text{nJ}$$

If we assume all this work is converted into heat, the resulting temperature increase ΔT in a hemispherical drop of 500nl is

$$\Delta T = \frac{5.9\text{nJ}}{500 \text{ x } 10^{-9} \text{ kg x } 4184 \frac{\text{J}}{\text{kgK}}} = 3\ \mu\text{K}$$

It is then reasonable to state that, using a ‘safety factor’ of 10 (accounting for the imperfections of this simplified model), an upper limit for the estimated temperature increase is about 30 µK.

References:
G.K. Batchelor, “An introduction to fluid dynamics”, Cambridge University Press, 1967.
S.F. Hoerner,” Fluid-dynamic drag: practical information on aerodynamic drag and hydrodynamic resistance”, Hoerner Fluid Dynamics, 1965.

Calculation of protein bound to surface of stir bar

Each stir bar is a rectangular box with a surface area of 1.78x10^{-7} m^2 (thickness = 1.5x10^{-5} m, width = 2x10^{-4} m, length = 4x10^{-4} m). Assuming the proteins are roughly spherical, the following maximum binding of a protein monolayer to the stir bar is obtained:

Trypsin

Diameter ≈ 4.5x10^{-9} m (PDB: 3MFJ), circular area = π(2.25x10^{-9}m)^2 = 1.59x10^{-17} m^2. Assuming the densest packing of equal diameter circles in a plane (Weisstein), the moles of trypsin bound would be

$$\frac{1}{6}\pi\sqrt{3} \times \frac{\left(\frac{1.78 \times 10^{-7}\,\mathrm{m}^2}{1.59 \times 10^{-17}\,\mathrm{m}^2}\right)}{6.022 \times 10^{23}\,\mathrm{mol}^{-1}} = 1.69 \times 10^{-14}\ \mathrm{mol}$$

For a 500 nl reaction, the concentration bound is

$$\frac{1.69 \times 10^{-14}\,\mathrm{mol}}{5 \times 10^{-7}\,\mathrm{l}} = 3.37 \times 10^{-8}\,\mathrm{M}$$

Human serum albumin

Diameter ≈ 6.5x10^{-9} m (PDB: 1BM0), circular area = π(3.25 x10^{-9}m)^2 = 3.32x10^{-17} m^2. Assuming the densest packing of equal diameter circles, the moles of HSA bound would be

$$\frac{1}{6}\pi\sqrt{3} \times \frac{\left(\frac{1.78 \times 10^{-7}\,\mathrm{m}^2}{3.32 \times 10^{-17}\,\mathrm{m}^2}\right)}{6.022 \times 10^{23}\,\mathrm{mol}^{-1}} = 8.08 \times 10^{-15}\ \mathrm{mol}$$

For a 500 nl reaction, the concentration bound is

$$\frac{8.08 \times 10^{-15}\,\mathrm{mol}}{5 \times 10^{-7}\,\mathrm{l}} = 1.62 \times 10^{-8}\,\mathrm{M}$$

Reference:
Weisstein, Eric W. "Circle Packing." From MathWorld--A Wolfram Web Resource.
http://mathworld.wolfram.com/CirclePacking.html